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Comparison of tools for the sustainability assessment of nanomaterials

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Abstract

Nanomaterials are becoming widely used in areas such as biomedical applications, food, environmental protection, energy production, information technology and agriculture. As such, more research has been conducted on their synthesis and manufacturing from a variety of feedstocks. However, concerns regarding their impact on human health and the environment leads researchers to conduct a variety of 'sustainability' assessments. The purpose of this paper was to review the current opinion of sustainability assessments concerning nanomaterials. Major assessment tools were reviewed including life cycle assessment, risk assessment and multi-criteria decision analysis, along with subcategories. The review found that each assessment tool did positively contribute to sustainability assessments, but each also had drawbacks of varying degrees. In particular, multi-criteria decision analysis provides the most relevant tool for conducting a sustainability assessment as it can handle criteria of any typology and provide multiple types of decision recommendations, including rankings, scores and classifications.

Keywords

Multi-criteria decision analysis (MCDA); risk assessment (RA); life cycle assessment (LCA); nanomaterials; sustainability assessment

1 Introduction

The rate at which potential risks are identified to areas such as the environment, society and health have been shown to not keep up with progress in the development of nanomaterials [1–6]. Reliance on methods from existing industrial processes must change to ensure a successful future of nanotechnology [7]. Research into risk assessments, sustainability and development of nanomaterials requires structured decision-making, to yield an optimal final strategy [8–10].

In order to give a complete consideration of both risks and impacts in the rapidly developing area of nanomaterials, there is a pressing need to combine current decision-making strategies with current assessment tools [11]. Investment in time, detail, a lack of data and no widely acknowledged definition of sustainability regarding nanomaterials means that, despite their presence in several sectors, nanomaterial-integrated products are marketed without full regulation [1–3,11–13].

The aim of this review is to provide an overview to the current methods used to assess risk and sustainability in nanomaterial life cycle and support comprehensive assessments. Using critical analysis of these methods, future directions for how these assessment methods should be approached are proposed.

2 Current tools

The process of selecting the correct tool for conducting a sustainability assessment could follow three stages as presented in Figure 1.[2,5,7,9,14–25] The first one devoted to the identification of the conceptual sustainability criteria according to the objective of the study. These criteria can be grouped into six broad groups, as has been identified by Cinelli *et al.* with respect to nanoproducts, including nanomaterials (Figure 2).[9]

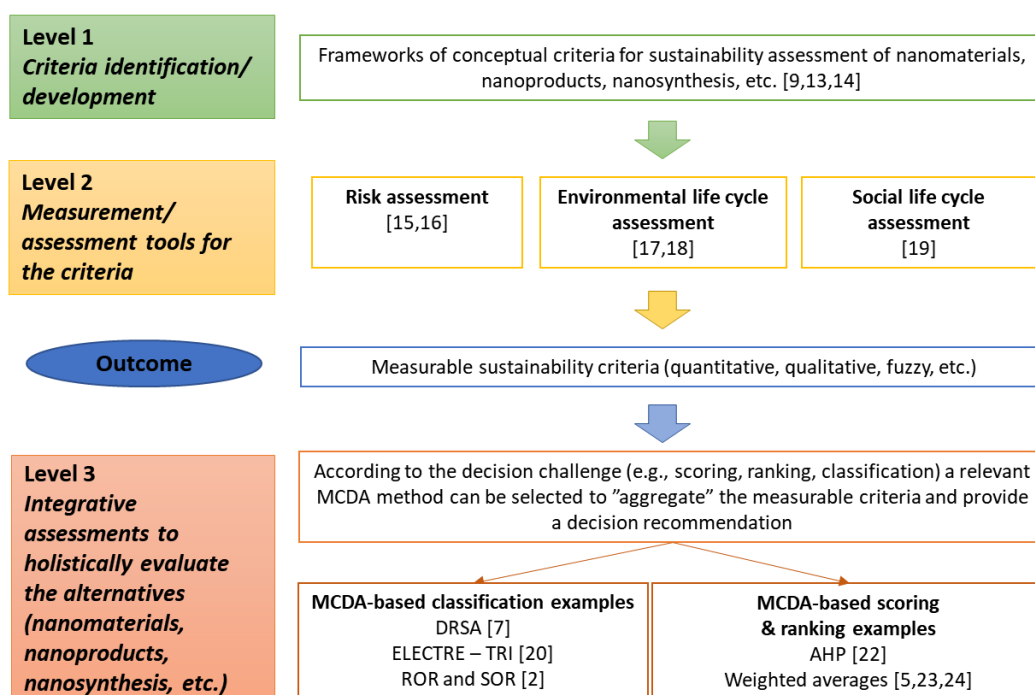


Figure 1 – Proposed methodology for holistic sustainability assessment of nanomaterials

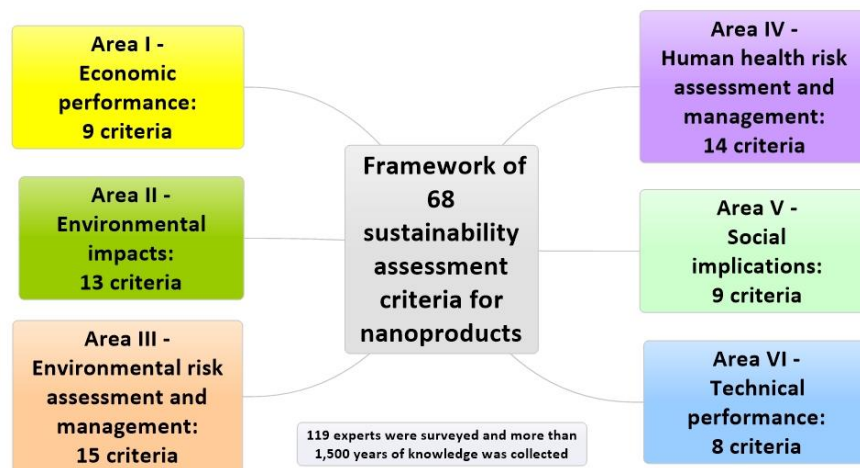


Figure 2 - Framework of sustainability assessment criteria for nanoproducts (from [9]). Reproduced under a CC BY 4.0 license.

The second stage consists in the identification of the tools to measure and provide an assessment for the conceptual criteria into a measurable format, which can be in different measurement unit, like quantitative, qualitative, fuzzy or another one. Generally accepted methodologies for investigating these include life cycle costing (LCC), risk assessments (RA), and life cycle assessments (LCA). The latter two of these will be explored in more detail within the context of nanomaterials in sections 2.1 & 2.2; whilst economic assessment is important within an industrial setting, the tools and techniques to assess LCC are already well established.[26]

The third level of the decision support is grounded on matching the decision challenge, namely the desired recommendation to be provided to the decision makers, being a score, a rank or a class of the alternatives under evaluation. According to the decision challenge, the relevant MCDA has to be selected or developed. Section 3 provides some examples of how our group as well as other researchers have implemented this strategy.

2.1 Life cycle assessment

Life Cycle Assessment (LCA) is a methodology that assesses the impact on the environment of product systems [27] by considering multiple environmental issues [28]. LCA is standardised according to the ISO 14040 series, using a four-stage structure [29]:

- 1) Goal and scope definition
- 2) Life cycle inventory (LCI) analysis
- 3) Life cycle impact assessment (LCIA)
- 4) Interpretation

These sections are highly variable according to the application of the LCA [30]. One opinion is that the very beginning of an LCA is the most important factor in obtaining results with the least variability and uncertainty [31]. This originates from deciding the goal, scope and boundary conditions of the system, determining the steps following it and in particular, the quantity of materials, energy flows and differences in the levels of nanoparticles released.

Alternatively, it can be argued that the most relevant phases to society of an LCA are use and end-of-life. However, LCAs are often conducted within a system boundary only including the manufacturing of the nanoproduct to the factory gate, omitting the use and end-of-life stages [27,28,32]. As described by Feijoo *et al.*, the consensus is that nanomaterials should be evaluated over their entire lifetime, so that the LCA can identify the risks from nanomaterials before they've been established [33]. Additionally, in the LCIA, the factors being considered are not specific to nanomaterials or their (eco)toxicological effects, making the LCIA inconclusive [27].

LCAs for nanoparticles are often missing the points at which nanoparticles are released during the complete life cycle, and as such they are not assessing them by ecological relevance [31]. Some reasoning behind leaving out these

stages in the LCA is due to lack of knowledge of their long-term impact on the environment during use and disposal [27], unknown effects on the environment and human health [28], and incomplete data about the use of nanoproducts.

This issue of lack of data also affects LCIs [7]; data is needed to make the LCI as accurate as possible for nanomaterials [31]. As such, a key limitation of inventory data is that many studies on LCA of nanomaterials are based on generic data since primary data on processes involving ENMs are not openly available [19,34]. However, one sector where the LCA of the use phases of nanomaterials has been studied is consumer goods; it is suggested that improved performance (specifically durability) gives a lower impact for the overall product [34,35].

Only for a small number of specific nanomaterials and manufacturing processes associated with nanomaterials does there exist quantitative data [27], making LCAs of nanomaterials on the whole difficult to conduct effectively. Hence, there is a pressing necessity for data to be made widely available in order to extend LCAs from cradle-to-gate to cradle-to-grave [32]. Moreover, data based on industry data is required, not adapted from literature or estimated from alternative sources [36]. Nanomaterials do not scale up in the same way that other materials do due to their composition, so simple numerical estimates provide an inaccurate environmental impact.

A detailed study of uncertainty quantification has recently been published [31], looking at the effects that uncertainty on the (i) functionality; (ii) LCI data; (iii) releases of nanoparticles and (iv) impact assessment. The authors found that the first step of LCA (i.e. goal and scope) which drives the selection of functionality, has the widest effect on the variability of the results.

However, several barriers to conducting a LCA still remain. Information available to individual purchasers can affect the success or failure of a NP, as they have the power to choose whether to purchase [37]. In particular, the perception of nanotechnology is susceptible to manipulation from both those for and against the use of NPs, and therefore to avoid a backlash, data can be difficult to obtain. Conversely, companies should be as transparent as possible on their activities involving NPs, ensuring good information flow to the public and relevant institutions in order to develop safe and responsible products [38]. These research findings indicate that only the engagement of all interested parties, including universities, industry, governmental organizations and the general public can effectively contribute to a widespread and agreed deployment of nanotechnology.

2.2 Risk assessments

An important area of nanoparticle assessments is understanding the impact on human health and the surrounding environment. Risk Assessment (RA) is one method used to focus on the toxicity of specific chemicals [28]. RA is based on hazards, effects and exposure assessment. In terms of evaluating the effects, alternative testing strategies are still under development, which indicates that quantitative and reliable effects data are still some way off. There is also the issue of exposure assessment which is still at a premature stage. There are not yet reliable measurements of nanomaterials concentration levels in working settings. This indicates that semi-quantitative RAs are going to be common for industry-wide NPs.

In any event, conventional approaches to assessing the hazard and suggesting alternatives are unable to differentiate for the different outcomes in toxicity due to slight variances in physical properties. General assessments can be conducted for individual endpoints, but cannot be transferred across to multiple endpoints. Whilst useful, this significant limitation should be noted [25]. Combined with the lack of information on economic and environmental impacts, risk assessments alone are not thorough enough but they can be effective when combined with LCA and Life Cycle Costing (LCC) to produce Life Cycle Sustainability Assessments.

3 Integrated sustainability assessments

One of the drawbacks of focusing purely on LCA is that the oft-discussed midpoint indicators are simply estimates of potential impacts, frequently carried out in a retrospective manner. More comprehensive frameworks have

previously been proposed [9,39–41]. In addition, LCA, RA and other tools have each been advanced for a specific scope. Consequently, merging methods that are not designed for the same scope is irrelevant [42]. By integrating the results of the assessments using multi-criteria decision analysis (MCDA), the scope can remain consistent across all of the tools. The emphasis is on the importance of the decision challenge in driving the selection/development of the relevant MCDA.

3.1 Multi-criteria decision analysis

MCDA has been suggested as an ideal process for conducting sustainability assessments, particularly in the area of NPs [9,43]. All the studies conducted so far using MCDA for sustainability assessment of NPs integrate the performance of NPs expressed as evaluation criteria to provide decision support for the user. Depending on the type of decision problem, an MCDA model is developed to provide the most relevant recommendation, usually in the form of a performance score, a ranking or classification [2,43,44] (see also Level 3 in Figure 1). Criteria of various sustainability pillars are characterised by different type and scale, such as qualitative, quantitative, fuzzy, continuous or discrete. Such heterogeneous parameters have been aggregated through MCDA approaches as a result of their unique capacities of accepting this typology of input.

MCDA processes identify potential alternatives (usually from experts) and decision criteria (usually from DMs/stakeholders), examine the performance of each alternative with respect to those criteria, and hence investigate priorities (from both the DMs and stakeholders) within the (possibly incomparable) criteria [1].

Following this idea, Cinelli *et al.* considered instead life cycle sustainability assessments (LCSA) [45]. The authors identified a comprehensive set of 68 criteria to assess the sustainability of nanoproducts (including NPs) by covering six main areas developed from the three pillars of sustainability thinking. These include environmental impacts, environmental risk assessment, human health risk assessment, social implications, economic performance as well as technical performance. According to the decision challenge, analysts can select the criteria that fit with their problem, moving from a single-domain to a multi-domain evaluation.

This idea has also been presented by Hicks, where textiles with different nanosilver concentrations and loss rates were assessed by aggregating the environmental costs (i.e. LCA) and the benefits (i.e. their antimicrobial efficiency) [23]. A score was derived through a simple weighted average and it was used to score and rank the textiles.

LCC methods quantify economic factors, by looking at a product's life cycle and noting the costs at each point whilst moderating the viewpoints of the stakeholders [30,46]. It was also noted how the social aspects of this method are hard to assess, as quantifying methods and data are lacking in this area [45]. One way of combining these assessments is MCDA, where methods can be categorised into three main theories; a utility function, an outranking relation and sets of decision rules [47,48].

3.1.1 Dominance-based Rough Set Approach (DRSA)

DRSA was used to devise a classification model based on decision rules [7,49], classifying synthesis protocols used for nanoparticles into green chemistry-based performance classes, through the combination of expert's knowledge and available information in peer-reviewed literature; these classifications result from a set of logical statements in the form of "if ..., then ..." rules [7]. DRSA can identify potential trade-offs that are being considered subconsciously by the DM based on the criteria used [50]. It does not require any data transformation, which is particularly useful when the data comes in both qualitative and quantitative form and it does not require any laborious weights elicitation from the DMs [43]. The drawback of DRSA is that the general software used in this area can only process one decision at a time so comparisons or alterations to classifications and rankings must be run independently [43].

3.1.2 Elimination and Choice Expressing the Reality (ELECTRE)

From outranking relation theory [43], ELECTRE are methods based on preference aggregation which operate by comparing alternatives pairwise using four binary relations; indifference, preference, weak preference and incomparability, with aims to establish whether one option is at least as good as another [43]. Cinelli *et al.* [21]

developed ELECTRE models for the green chemistry-based synthesis of silver nanoparticles by providing uncertainty-characterised performance classes. The paper looked specifically at comparing the results of ELECTRE with DRSA to assess their concordance. The comparison provided assurance that these methods aid decision making in an easy-to-understand manner and also provide consistent classifications [21]. Whilst this paper is specific to silver nanoparticles, the idea is easily adaptable to comparing other methods for other nanoparticles. However, ELECTRE methods have the drawback that they exploit only the ordinal character of the data, hence they are not capable of accounting for the extent in the difference of performance.

3.1.3 Analytical Hierarchy Process (AHP)

AHP is an MCDA method based on pairwise comparisons providing a single score for each alternative and it takes all the factors of a decision problem into account by means of a criteria hierarchy [22,43]. Topuz *et al.* [22] investigated the environmental risk assessment of nanomaterials using AHP and fuzzy interference rules. **This assessment involved** looking into the life-cycle of the product from production to end-of-life so that all potential release pathways of nanoparticles into the environment can be identified and categorized by experts. The pairwise comparison means that AHP can be limited as a stand-alone technique, but it can be combined with fuzzy set theory or mathematical programming, yielding decisions that are more realistic [51]. There is also no possibility of using thresholds in the AHP methodology [43].

4 Conclusion

The contributions of LCA, RA and MCDA tools vary depending on which pillar is being considered, with MCDA being the only methodology capable of covering all aspects of sustainability. This is in part due to the flexibility of MCDA allowing to include any type of criteria depending on the product/process, and the limited set of criteria that can be analysed by LCA and RA. LCA studies are data intensive and they have mostly not covered the end-of-life phase of a NP life cycle. RA only covers environmental and human toxicity effects. MCDA-based assessments can include economic, social and environmental impacts and also integrate them in a comprehensive, transparent and easy to understand evaluation for each alternative (e.g., NP) under study.

However, in order for these tools to become effective at producing a reliable and informative analysis, data is required from practitioners that is ideally based on real observations. In the industrial setting, it should cover both technological effectiveness as well as economic suitability rather than assumptions based on potentially unrelated literature or prior knowledge. A combined focus across all three pillars of sustainability is required as all too often there is a bias from academia towards the environmental benefits and impacts which reduces the overall impact when trying to reach industry. Strong collaborations will need to be forged across sectors in order for this goal to be realised.

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Using a stochastic version of an MCDA classification method, the authors demonstrate that a robust green chemistry-based performance class can be assigned to synthesis processes for silver nanoparticles. This is the first study to combine experts' judgement with peer-reviewed literature to assess the "greenness" of nanosynthesis processes

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